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## **Report Title**

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## Towards direct simulations of counterflow flames with consistent numerical differential-algebraic boundary conditions

*P. D. Kourdis<sup>1</sup> and J. Bellan<sup>1,2</sup>*

<sup>1</sup>*California Institute of Technology, Pasadena, California 91125, USA*

<sup>2</sup>*Jet Propulsion Laboratory, California Institute of Technology, Pasadena, California, 91109-8099, USA*

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**Keywords:** *two-dimensional counterflow flames; high-pressure counterflow flames*

### 1 Introduction

The counterflow configuration provides a comprehensive framework for studying the characteristics of non-premixed laminar and turbulent flame problems [1, 2, 3, 4, 5, 6]. However, apart from the simplified one-dimensional spatial models, the fidelity of direct numerical simulations (DNSs) for the counterflow configuration in terms of robustness/accuracy exhibit significant sensitivity to the boundary condition (BC) treatment [7, 8, 9]. This behavior is mainly due to the multi-directional character of the flow at the boundaries which must be properly accounted by the BCs. To mitigate this problem, Yoo et al. [7] developed improved BCs based on the Navier-Stokes Characteristic Boundary Conditions [10] (NSCBCs) for laminar and turbulent counterflow flames. The major improvement consisted in introducing the (no-longer negligible) transverse terms into the Locally One Dimensional Inviscid (LODI) relations in order to capture the multi-dimensional effects at the inflow/outflow boundaries. However, two major shortcomings can also be identified with the improved NSCBCs. First, they preserve the use of relaxation coefficients entering the improved LODI relations and these coefficients are problem specific. These coefficients provide an optimal balance between maintaining the prescribed upstream values for the inflow variables and reducing spurious wave reflections, and usually must be determined through a trial and error process; this is an expensive, time-consuming procedure. Second, once derived for real-gas, the implementation of these revised NSCBCs adds a considerable computational cost.

In this work, we adopt a totally different approach for constructing BCs for the counterflow configuration that results in a very concise framework. In particular, we combine the steady-state Navier-Stokes equations with an initial flow of potential type to construct numerically consistent

algebraic BCs at the inflow boundaries. The structure of the paper is as follows. First, the governing equations of the problem are presented. A detailed discussion on the construction of the initial profile of the flow follows. Then, the new inflow and outflow boundary conditions are provided. The specifics regarding the numerical implementation follows. Next, the validation of the proposed numerical differential-algebraic BCs is performed. Finally, a summary is given.

## 2 Governing Equations

### 2.1 The Navier-Stokes equations

The Navier-Stokes (NS) equations for a compressible reacting multicomponent mixture of  $N$  species expressed in terms of the conservative variables  $\tilde{\mathbf{U}} = [\tilde{U}_m] (m = 1, \dots, N + 4)$  can be cast in compact form as

$$\frac{\partial \tilde{\mathbf{U}}}{\partial t} + \frac{\partial \mathbf{F}^i}{\partial x_i} = \tilde{\mathbf{C}}, \quad (1)$$

where  $\mathbf{F}^i = [F_m^i] (m = 1, \dots, N + 4)$  denotes the flux vector of the conservative variables along the  $i$ -th direction, i.e.

$$\mathbf{F}^i \equiv [\rho u_i, \rho u_1 u_i + p \delta_{1i}, \rho u_2 u_i + p \delta_{2i}, \rho u_3 u_i + p \delta_{3i}, \rho u_i Y_1, \dots, \rho u_i Y_{N-1}, (\rho e_t + p) u_i]^T, \quad (2)$$

and the vector  $\tilde{\mathbf{C}} = [C_m] (m = 1, \dots, N + 4)$  is defined as

$$\tilde{\mathbf{C}} \equiv [0, \frac{\partial \tau_{1j}}{\partial x_j}, \frac{\partial \tau_{2j}}{\partial x_j}, \frac{\partial \tau_{3j}}{\partial x_j}, -\frac{\partial J_{1j}}{\partial x_j} + \dot{\omega}_1, \dots, -\frac{\partial J_{N-1j}}{\partial x_j} + \dot{\omega}_{N-1}, -\frac{\partial q_j}{\partial x_j} + \frac{\partial (\tau_{ij} u_i)}{\partial x_j}]^T. \quad (3)$$

The usual notation applies in that the indices  $i$  and  $j$  follow the summation convention,  $t$  is time,  $x_j$  is the  $j$ -th spatial coordinate,  $\rho$  is the mass density of the fluid,  $u_j$  is the  $j$ -th component of the velocity vector,  $Y_n$  is the mass fraction of species  $n$ ,  $p$  is the pressure,  $e_t = e + \frac{1}{2} u_i u_i$  is the total specific energy ( $e$  denotes the specific internal energy),  $J_{nj}$  is the  $j$ -th component of the mass flux vector  $\mathbf{J}_n$  of species  $n$ ,  $q_j$  is the  $j$ -th component of the heat flux vector  $\mathbf{q}$  and  $\dot{\omega}_n$  is the mass reaction rate of species  $n$ . Finally,  $\tau_{ij}$  is the Newtonian viscous stress tensor

$$\tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right), \quad (4)$$

where  $\mu$  is the dynamic viscosity of the mixture and  $\delta_{ij}$  is the Kronecker delta. Body forces have been neglected in the present equations.

The species-mass and heat fluxes have been given in detail elsewhere [11] and their expressions are based on the fluctuation-dissipation theory [12, 13, 14]. The mixing rules employed for the computation of the mass diffusion coefficients and thermal diffusion factors have been derived by Harstad and Bellan [15] and are based on the conjunction of nonequilibrium thermodynamics [12] in the limit of low pressure and Grad's 13-moment theory [16].

### 2.2 Transport properties

Transport properties were computed according to the most up-to-date methods [15, 17, 18, 19], an example being provided in Masi et al. [11].

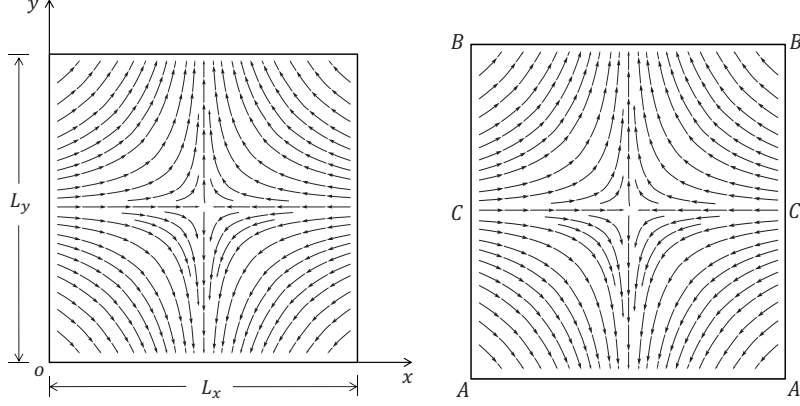


Figure 1: The initial potential flow entering through both the left  $AB$  and right  $A'B'$  inlet boundaries, and exiting through the  $AA'$  and  $BB'$  boundaries. The solid lines represent the streamlines and the arrows show the direction of the flow.

### 2.3 Equation of state

All NS equations are coupled with the Peng-Robinson (PR) equation of state (EOS) [20]

$$p = \frac{R_u T}{v_{PR} - b_{mix}} - \frac{a_{mix}}{v_{PR}^2 + 2b_{mix}v_{PR} - b_{mix}^2} \quad (5)$$

from which  $T$  and  $p$  are obtained as an iterative solution of two nonlinear equations that satisfy both the values of  $\rho$  and  $e$  as obtained from the solution of the conservation equations. In the PR EOS,  $v_{PR}$  is the PR molar volume and the molar volume  $v = v_{PR} + v_s$  where  $v_s$  is the volume shift computed to improve the accuracy of the PR EOS for high-pressure conditions [21], while the terms  $a_{mix}$  and  $b_{mix}$  are functions of  $T$  and  $X_i$  [11].

### 3 Initial profile: Inviscid incompressible potential flow

The initial profiles correspond to a two-dimensional potential flow in which two opposing streams, each of constant density and composition, are injected from the two boundaries  $AB$  and  $A'B'$  of length  $L_y$  in the  $x$ -direction; the streams exit the domain through the two boundaries  $AB$  and  $A'B'$  of length  $L_x$  at the  $y$ -direction as illustrated in Fig. 1. Reference quantities (subscript  $ref$ ) constant in time are first specified at the left (superscript  $l$ ) and the right (superscript  $r$ ) boundary points  $C$  and  $C'$ . The reference pressures at the two inlets are set  $p_{ref}^l = p_{ref}^r = p_{ref}$ , so that for the initial flow, the stagnation point (S) is always located at the centerline with  $x_S = L_x/2$  and also  $y_S = L_y/2$ .

The initial density and mass fraction fields are given as

$$[\rho^0(x, y), Y_n^0(x, y)] = \begin{cases} [\rho_{ref}^l, Y_{n,ref}^l] & \text{if } 0 \leq x < L_x/2, \forall y \\ [\rho_{ref}^r, Y_{n,ref}^r] & \text{if } L_x/2 < x \leq L_x, \forall y \end{cases}, \quad (6)$$

where a discontinuity arises in  $\rho^0(x, y)$  and  $Y_n^0(x, y)$  at  $x = L_x/2, \forall y$  when  $\rho_{ref}^l \neq \rho_{ref}^r$  and

$Y_{n,ref}^l \neq Y_{n,ref}^r$ . The components of the initial velocity field are

$$u_x^0(x, y) = -\frac{2\kappa(x - L_x/2)}{1 + \sqrt{\rho_{ref}^l/\rho_{ref}^r}}, \quad 0 \leq x < L_x/2; \quad u_x^0(x, y) = -\frac{2\kappa(x - L_x/2)}{1 + \sqrt{\rho_{ref}^r/\rho_{ref}^l}}, \quad L_x/2 < x \leq L_x \quad (7)$$

$$u_y^0(x, y) = \frac{2\kappa(y - L_y/2)}{1 + \sqrt{\rho_{ref}^l/\rho_{ref}^r}}, \quad 0 \leq x < L_x/2; \quad u_y^0(x, y) = \frac{2\kappa(y - L_y/2)}{1 + \sqrt{\rho_{ref}^r/\rho_{ref}^l}}, \quad L_x/2 < x \leq L_x \quad (8)$$

where  $\kappa$  is the strain rate.  $u_x^0(x, y)$  is continuous  $\forall(x, y)$ , while  $u_y^0(x, y)$  has a discontinuity at  $x = L_x/2, \forall y$  when  $\rho_{ref}^l \neq \rho_{ref}^r$ .

Using (i) the common reference pressure,  $p_{ref}$ , of points  $C$  and  $C'$ , (ii) the Bernoulli equation which holds for inviscid incompressible flows and (iii) the fact that for irrotational (i.e. potential) flows the total pressure, as given by the Bernoulli equation, is the same for all points of the flow (otherwise the Bernoulli equation would only hold along a streamline), we obtain the initial pressure field,  $p^0$ , as

$$p^0(x, y) = p_{ref} + \frac{1}{2}\rho_{ref}^l \left[ (u_x^0(x_C, y_C))^2 + (u_y^0(x_C, y_C))^2 \right] - \frac{1}{2}\rho_{ref}^l \left[ (u_x^0(x, y))^2 + (u_y^0(x, y))^2 \right], \quad (9)$$

for  $0 \leq x < L_x/2, \forall y$ , where  $x_C = 0$  and  $y_C = L_y/2$ , while for  $L_x/2 < x \leq L_x, \forall y$

$$p^0(x, y) = p_{ref} + \frac{1}{2}\rho_{ref}^r \left[ (u_x^0(x_{C'}, y_{C'}))^2 + (u_y^0(x_{C'}, y_{C'}))^2 \right] - \frac{1}{2}\rho_{ref}^r \left[ (u_x^0(x, y))^2 + (u_y^0(x, y))^2 \right], \quad (10)$$

where  $x_{C'} = L_x$  and  $y_{C'} = L_y/2$ .

By construction, the initial potential flow satisfies the steady-state incompressible Euler's equations. The availability of  $p^0(x, y), \rho^0(x, y), Y_1^0(x, y), \dots, Y_N^0(x, y)$  in conjunction with the EOS allows the determination of the initial temperature field of the flow,  $T^0(x, y)$ . With the calculated  $T^0(x, y)$ , the initial specific internal energy field is obtained. It follows that the initial field of conservative variables,  $\tilde{U}^0(x, y)$ , can then be readily constructed.

Finally, we note that for the counterflow configuration the use of a potential flow as initial flow is consistent with the fact that even when starting computations with a plug flow (i.e. zero  $y$ -components of the velocity vector at the inlets), the flow quickly converges to a potential type.

## 4 Boundary conditions

### 4.1 Inflow boundary conditions

Instead of explicitly imposing timewise constant boundary values (also known as hard BCs) for the conservative variables at the two inlets  $AB$  and  $A'B'$ , we impose the steady-state NS compressible form of the conservation equations for  $\rho, \rho u_x, \rho u_y, \rho Y_1, \dots, \rho Y_{N-1}$ . Using these equations as BCs means that the initial values imposed on the inlets  $AB$  and  $A'B'$  for these variables are implicitly constrained to be constant with time. Most importantly, the transverse terms that give rise to multi-directional effects at the inflow boundaries are inherently present in the BCs. In addition to the above BCs, the thermodynamic computation of the energy  $\rho e_t = \rho \bar{e}_t(T(x, y), p(x, y), Y_1(x, y), \dots, Y_N(x, y))$  is used for the boundary values of  $\rho e_t$  at the two inlets, where  $\bar{e}_t$  is calculated using the

current values of  $\rho, \rho u_x, \rho u_y, \rho Y_1, \dots, \rho Y_{N-1}$  and  $T$  is obtained from the EOS, so that the values of  $\rho \bar{e}_t$  are readily available.

By construction, the initial values of  $\rho, \rho u_x, \rho u_y, \rho Y_1, \dots, \rho Y_{N-1}$  at the inlets (see Section 3) satisfy the Euler instead of the NS steady-state equations. Since the inlet boundaries are usually located away from the flame, these initial values provide a good initial guess for the NS steady-state equations which can be corrected [22] to account the viscous and species mass-flux effects.

#### 4.2 Outflow boundary conditions

At the outflow boundaries  $A'A$  and  $BB'$ , the solution satisfies the unsteady compressible, reactive flow NS equations since the conditions there are the outcome of the processes taking place in the interior of the domain. At these boundaries we assume that  $p$  stays constant with time, taking the value initially provided by the Bernoulli equation.

### 5 Numerical scheme

An eight-order explicit finite-difference scheme is used for the spatial derivatives. After spatial discretization, the steady NS equations become algebraic equations at a node, whereas the unsteady NS equations become ordinary differential equations at a node. As a result, at the nodes of the inflow boundaries  $AB$  and  $A'B'$ , the BCs are numerically of algebraic type. In addition, auxiliary ghost points can be used from the left of the boundary  $AB$  and the right of the boundary  $A'B'$  (since the solution is known there) to enhance the finite difference approximation of the spatial derivatives in those equations. At the nodes of outflow boundaries  $A'A$  and  $BB'$ , the BCs are of differential type and one-sided finite differencing is used.

The resulting numerical system of differential-algebraic equations [23] is integrated in time with the differential-algebraic solver IDA of the SUNDIALS suite [24]. The integration method used in IDA is a variable-order, variable-coefficient BDF (Backward Differentiation Formula), in fixed-leading-coefficient form where the order of the method varies between 1 and 5. The BDF method can handle the stiffness introduced in the numerical integration of the NS equations due to the presence of chemical source terms. IDA supports parallel computations through the message passing interface (MPI) protocol and provides a routine that computes consistent initial conditions from a users' initial guess [22, 25].

### 6 Reproducing potential flows

To validate the proposed differential-algebraic BCs of Section 4, we consider two symmetric non-reacting potential flows where either  $H_2$  or  $O_2$  enters from both inlets. The goal is to numerically reproduce these two steady-state potential flows at computational times characteristic to reaction/diffusion problems.

Table 1: Inflow conditions at  $C$  and  $C'$  (see the right part of Fig. 1) for two  $H_2$  and one  $O_2$  simulations.  $N_x$  and  $N_y$  are the number of points in the  $x$  and  $y$  directions.  $L_x = L_y = 10$  mm.

Case	Species	$\rho_{ref}$ (kg/m <sup>3</sup> )	$T_{ref}$ (K)	$p_{ref}$ (bar)	$\kappa$ (s <sup>-1</sup> )	$N_x$	$N_y$
A	H <sub>2</sub>	0.08077	300	1	$2 \times 10^3$	104	104
B	H <sub>2</sub>	0.08077	300	1	$4 \times 10^3$	144	144
-	O <sub>2</sub>	1.2837	300	1	$2 \times 10^3$	200	200

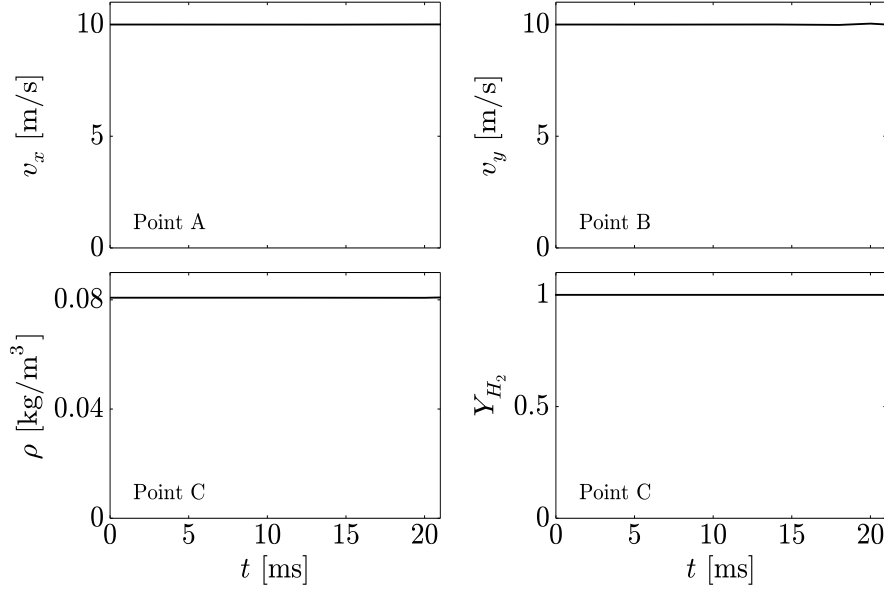


Figure 2: Temporal variation of  $\rho$ ,  $v_x$ ,  $v_y$ ,  $p$  and  $Y_{H_2}$  at inlet boundary points for Case A of Table 1. The labeling of the points refers to the right part of Fig. 1.

### 6.1 The H<sub>2</sub> symmetric potential flow

For the symmetric H<sub>2</sub> potential flow, the two situations considered differ in the imposed strain rates (see Table 1). Due to space constraints, we only show below the temporal variation of the inlet boundary points for case A (Fig. 2) and the spatial variation of primitive variables at  $t = 6$  ms for case B (Fig. 3). Figure 2 shows the temporal evolution of the boundary values of  $\rho$ ,  $v_x$ ,  $v_y$  and  $Y_{H_2}$  at points on the left inlet boundary; the prescribed initial boundary values are excellently maintained by the imposed NS steady-state BCs at the two inlets  $AB$  and  $A'B'$ . Figure 3 illustrates for case B the initial ( $t = 0$  ms) spatial variation of  $\rho$ ,  $v_x$ ,  $v_y$ ,  $p$  and  $Y_{H_2}$  for  $x$ -sections of the computational domain and the spatial variation of the same variables obtained at  $t = 6$  ms. Clearly, the steady-state potential flow is accurately reproduced numerically in all respects for the larger  $\kappa$  value.

### 6.2 The O<sub>2</sub> symmetric potential flow

For the symmetric O<sub>2</sub> potential flow the inflow conditions and computational mesh are given on Table 1. The results of the simulation for O<sub>2</sub> represent a simulation performed with a fluid having a density of  $\mathcal{O}(10)$  larger compared to that of H<sub>2</sub> used in the previous two simulations. The results are not illustrated, but they show the same high fidelity in maintaining the imposed initial potential flow as in the H<sub>2</sub> simulations.

## 7 Summary and conclusions

New BCs have been developed for the counterflow configuration that provide a very concise framework inherently accounting for the multi-directional character of the flow at the boundaries. Upon discretization of the steady-state NS equations, the BCs at the inflow boundaries are of algebraic type, whereas upon discretization of the unsteady NS equations, those at the outflow boundaries are of differential type. This formulation of the numerical BCs as differential-algebraic ones re-



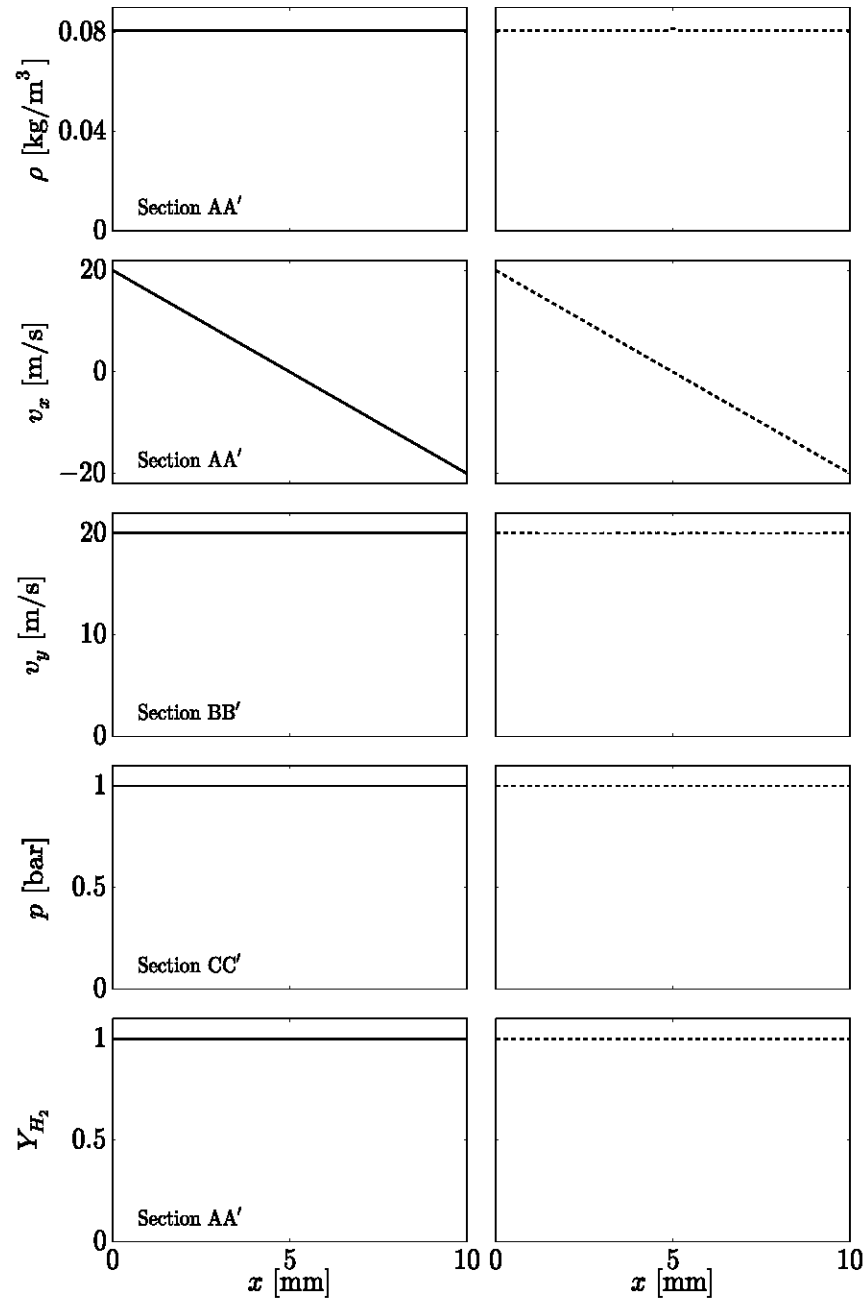


Figure 3: Spatial variation of  $\rho$ ,  $v_x$ ,  $v_y$ ,  $p$  and  $Y_{H_2}$  for Case B of Table 1. The labeling of the sections refers to the right part of Fig. 1. Left column:  $t = 0$  ms. Right column:  $t = 6$  ms.

quires the use of a numerical integration software capable of handling initial-value problems for differential-algebraic systems of equations [24].

For the non-reactive-flow validation of the differential-algebraic BCs, two symmetric non-reacting potential flows were considered with either  $H_2$  or  $O_2$  as injected species from both inlets. For  $H_2$ , two different strain rates cases were examined whereas for  $O_2$  only one strain rate flow is simulated. Irrespective of the species or the strain rate, the initial potential flow was reproduced with high fidelity over the entire computational domain without numerical artifacts, i.e. without use of dissipative filters or introduction of relaxation constants into the BCs.

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## Sub Topic: Laminar Flames

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